Conformational Analysis via Chirotope Generation

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Outline

Conformational analysis

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A chemical structure ...

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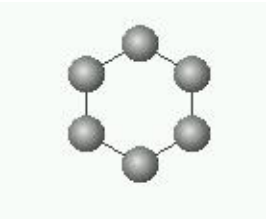

cyclohexane

Conformational analysis

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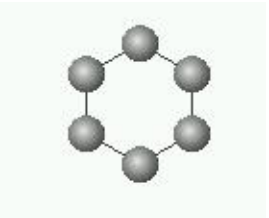

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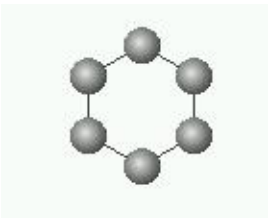

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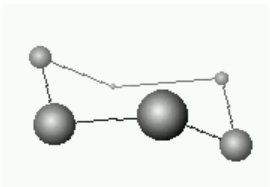
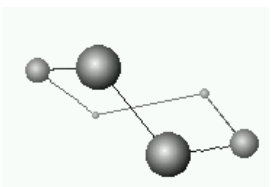


chair form



twisted form

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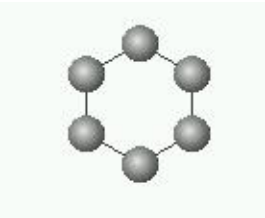

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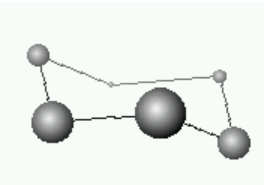

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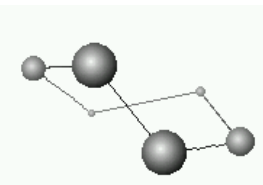


twisted form

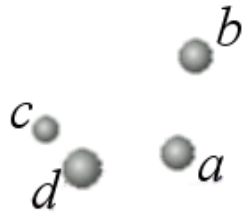
Definition

Under *conformer generation*, we understand the generation of a reasonably distributed sample of the conformation space.

The orientation function

The orientation function

- The "right-hand rule":



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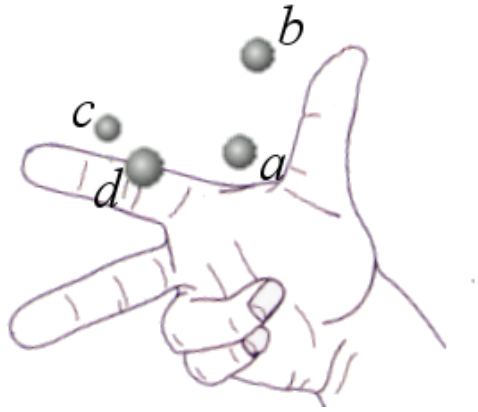

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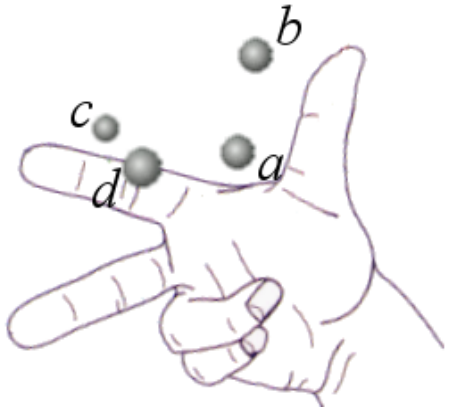

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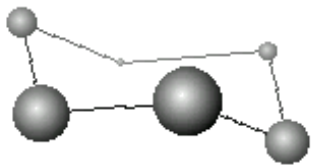

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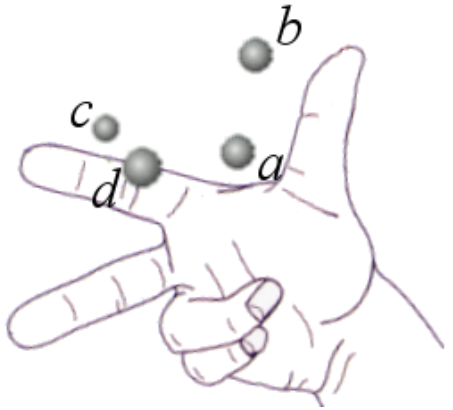

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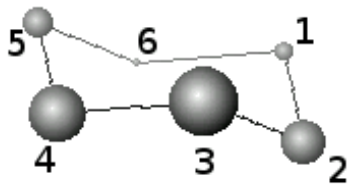

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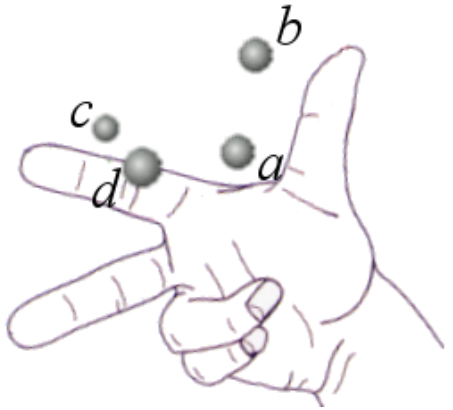

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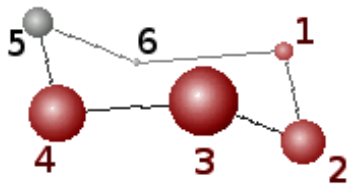

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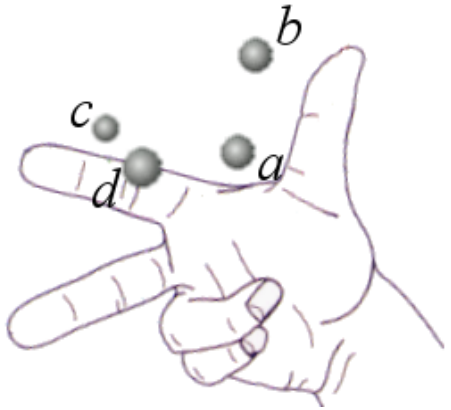

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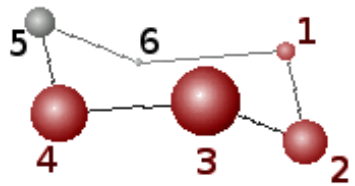

1234

+

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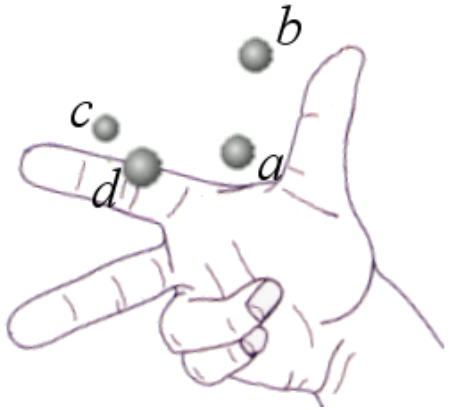

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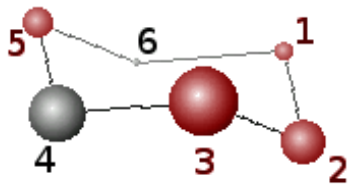

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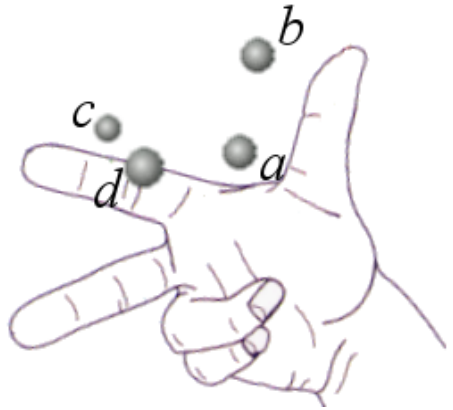

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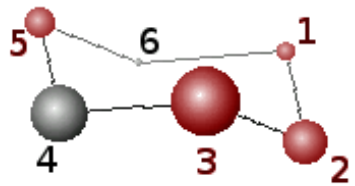

1234
1235

+ +

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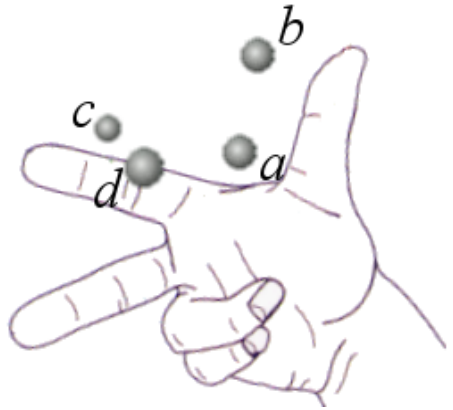

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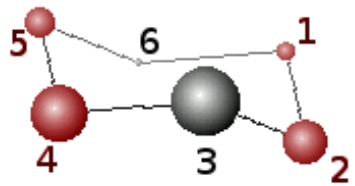

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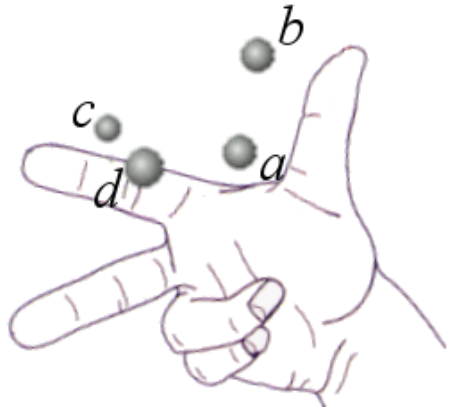

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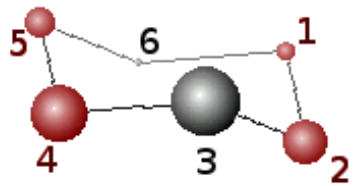

1234
1235
1245

$++0$

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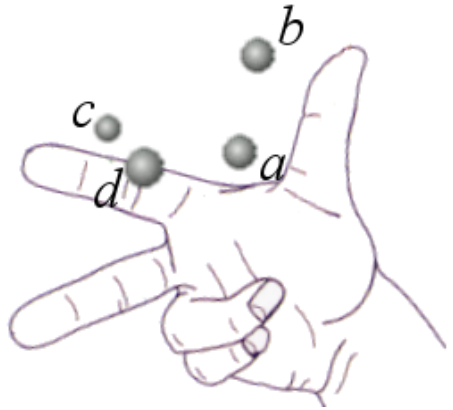

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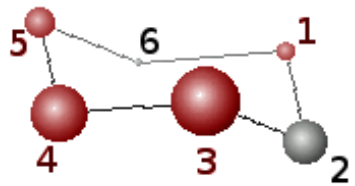

1234 1235 1245 1345

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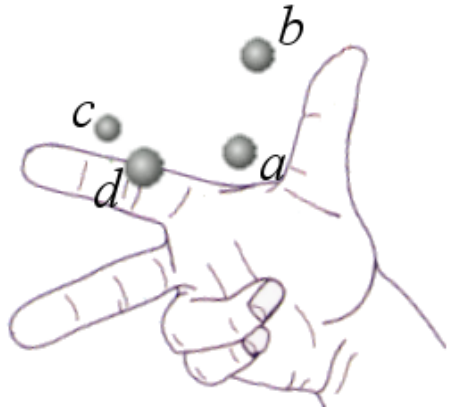

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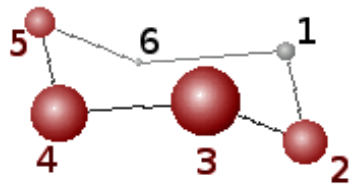

1234 1235 1245 1345 2345

$++0\ --$

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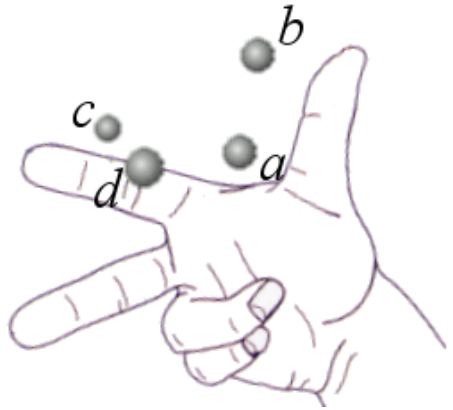

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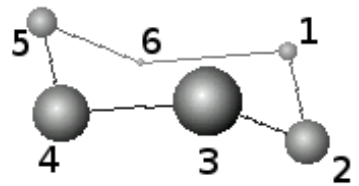

1234 1235 1245 1345 2345 1236 1246 1346 2346 1256 1356 2356 1456 2456 3456

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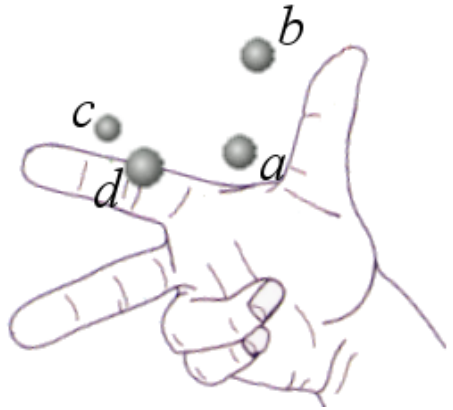

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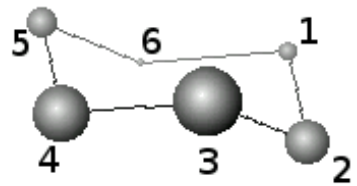

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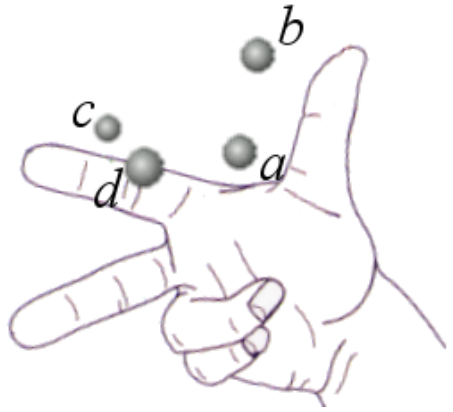

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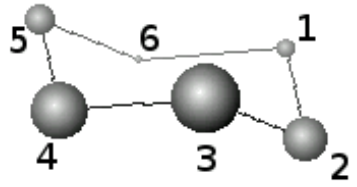

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The *orientation function* χ (in combination with the molecular graph) describes a molecule on an intermediate level between constitution and conformation.

Conformer generation

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- Generate mappings, which potentially are orientation functions.

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As potential orientation functions, we consider chirotopes.

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$$\chi : n^4 \rightarrow \{0, \pm 1\}$$

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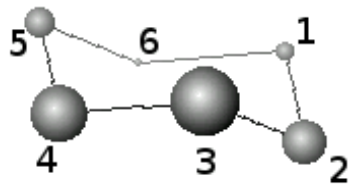
$$\chi(\vec{a}) \cdot \chi(\vec{b}) = 1 \Longrightarrow \exists i \in n : \chi(b_i, a_1, \ldots, a_3) \cdot \chi(b_0, \ldots, \underbrace{a_0}_{\substack{\uparrow \\ i\text{-th position}}}, \ldots, b_3) = 1\,. \qquad \text{(GP)}$$

Canonical forms of chirotopes



$$\begin{matrix} 1234 & 1235 & 1245 & 1345 & 2345 & 1236 & 1246 & 1346 & 2346 & 1256 & 1356 & 2356 & 1456 & 2456 & 3456 \end{matrix}$$

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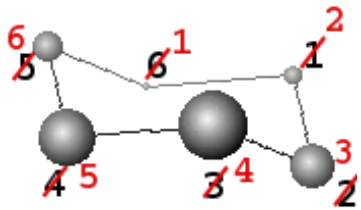

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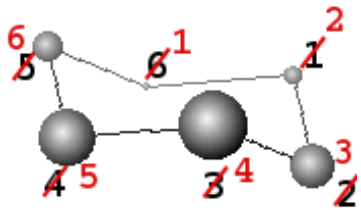

$$\chi = \begin{array}{cccccccccccccccccccc} 1234 & 1235 & 1245 & 1345 & 2345 & 1236 & 1246 & 1346 & 2346 & 1256 & 1356 & 2356 & 1456 & 2456 & 3456 \\ + & + & 0 & - & - & + & + & 0 & - & + & + & 0 & + & + & + \\ - & - & 0 & + & + & - & - & 0 & + & - & - & 0 & - & - & - \end{array}$$

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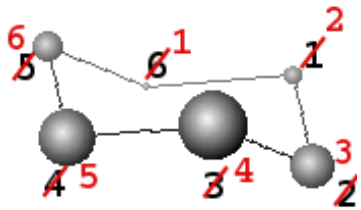

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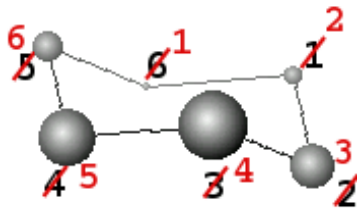
- Canonical forms are important for chirotopes (as they are for the molecular graphs).

Canonical forms of chirotopes



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- We are able to calculate the canonical form.

Radon partitions

- A chemical unfeasable conformation:

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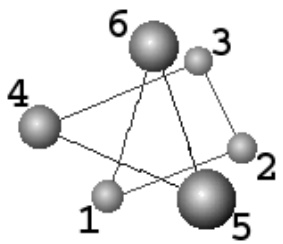

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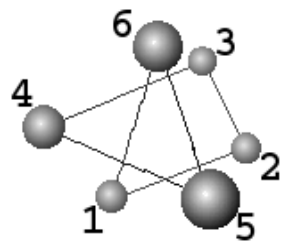

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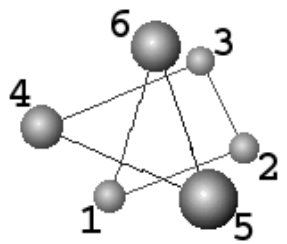

1234 1235 1245 1345 2345 1236 1246 1346 2346 1256 1356 2356 1456 2456 3456

$$\chi = + + + + + + + + + + - - + + + +$$

Question:

Is it possible to recognize the infeasibility from the orientation function only?

Radon partitions (2)

- A *radon partition* is a pair (A,B) of subsets of all atoms, such that their convex hulls intersect:

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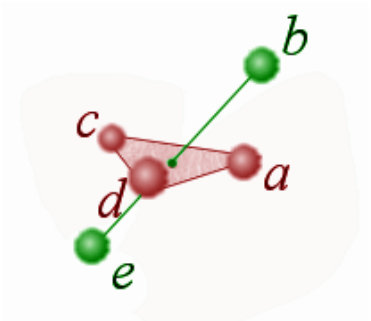

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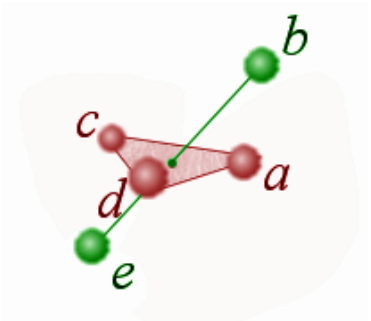

- The chirotope determines all radon partitions.

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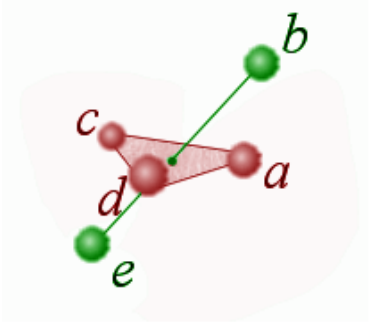
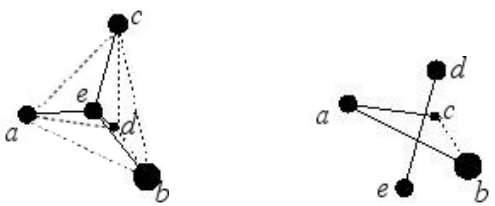
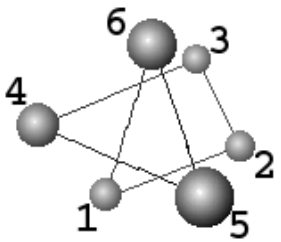


- The chirotope determines all radon partitions.
- This way, we can recognize (some) chemical unfeasable configurations, e.g.



Radon partitions

- A chemical unfeasable conformation:



1234 1235 1245 1345 2345 1236 1246 1346 2346 1256 1356 2356 1456 2456 3456

$$\chi = + + + + + + + + + + - - + + + +$$

Radon partitions

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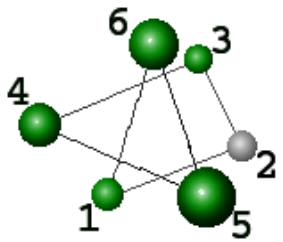

$$\begin{array}{c} 1234\,1235\,1245\,1345\,2345\,1236\,1246\,1346\,2346\,1256\,1356\,2356\,1456\,2456\,3456 \\ \chi = +\,+\,+\,+\,+\,+\,+\,+\,+\,-\,-\,+\,+\,+\,+ \end{array}$$

Radon partitions

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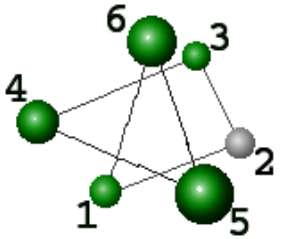

$$\chi = \begin{array}{cccccccccccccccc} 1234 & 1235 & 1245 & 1345 & 2345 & 1236 & 1246 & 1346 & 2346 & 1256 & 1356 & 2356 & 1456 & 2456 & 3456 \\ + & + & + & + & + & + & + & - & + & - & + & + & - & + & + \end{array}$$

Radon partitions

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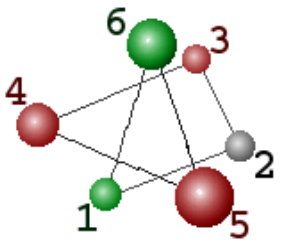

$$\chi = \begin{array}{cccccccccccccccccccc} 1234 & 1235 & 1245 & 1345 & 2345 & 1236 & 1246 & 1346 & 2346 & 1256 & 1356 & 2356 & 1456 & 2456 & 3456 \\ + & + & + & + & + & + & + & - & + & - & + & + & - & + & + \end{array}$$

Radon partitions

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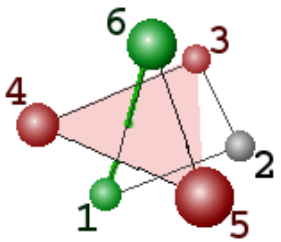

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Radon partitions

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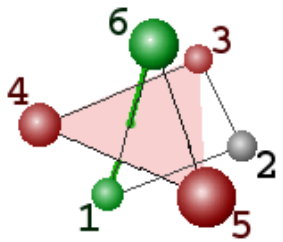
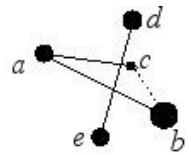


is of form



$$\chi = \begin{array}{ccccccccccccccc} 1234 & 1235 & 1245 & 1345 & 2345 & 1236 & 1246 & 1346 & 2346 & 1256 & 1356 & 2356 & 1456 & 2456 & 3456 \\ + & + & + & + & + & + & + & - & + & - & + & + & - & + & + \end{array}$$

Radon partitions

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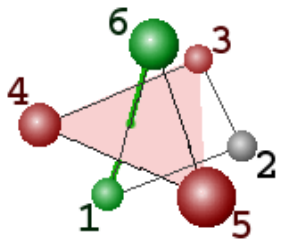

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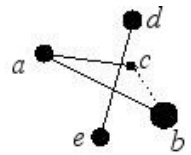
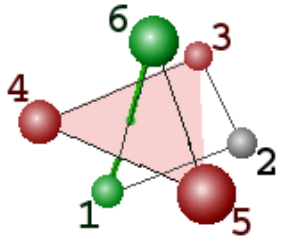


$$\chi = \begin{array}{cccccccccccccccc} 1234 & 1235 & 1245 & 1345 & 2345 & 1236 & 1246 & 1346 & 2346 & 1256 & 1356 & 2356 & 1456 & 2456 & 3456 \\ + & + & + & + & + & + & + & - & + & - & + & + & - & + & + \end{array}$$

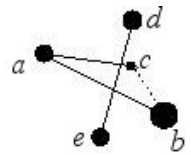
- We did not need coordinates nor angles for this test.

Radon partitions

- A chemical unfeasable conformation:



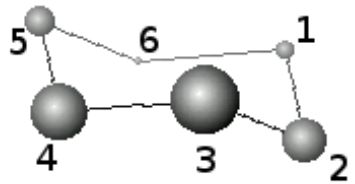
is of form



$$\chi = \begin{array}{ccccccccccccccc} 1234 & 1235 & 1245 & 1345 & 2345 & 1236 & 1246 & 1346 & 2346 & 1256 & 1356 & 2356 & 1456 & 2456 & 3456 \\ + & + & + & + & + & + & + & - & + & - & + & + & - & + & + \end{array}$$

- We did not need coordinates nor angles for this test.
- $\Rightarrow$ Efficient test during conformer generation.

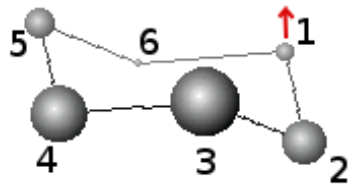
Partially defined chirotopes



$$\begin{matrix} 1234 & 1235 & 1245 & 1345 & 2345 & 1236 & 1246 & 1346 & 2346 & 1256 & 1356 & 2356 & 1456 & 2456 & 3456 \end{matrix}$$

$$\chi = ++0\ --++0\ -++0\ +++$$

Partially defined chirotopes



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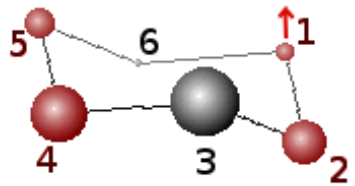

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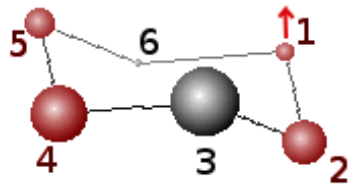

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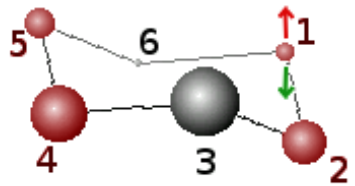

$$\begin{array}{c} 1234\,1235\,1245\,1345\,2345\,1236\,1246\,1346\,2346\,1256\,1356\,2356\,1456\,2456\,3456 \\ \chi = ++\emptyset^{+}\,--++0\;-++0\;+++ \end{array}$$

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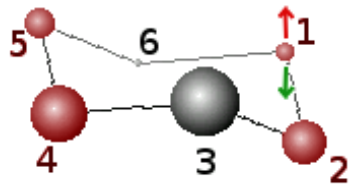

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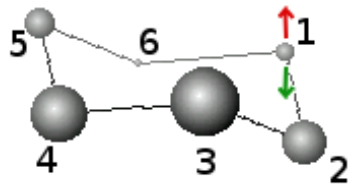

$$\begin{array}{l} \\ \chi = \\ \chi = \\ \chi = \end{array} \begin{array}{cccccccccccccc} 1234 & 1235 & 1245 & 1345 & 2345 & 1236 & 1246 & 1346 & 2346 & 1256 & 1356 & 2356 & 1456 & 2456 & 3456 \\ + & + & 0 & - & - & + & + & 0 & - & + & + & 0 & + & + & + \\ + & + & + & - & - & + & + & + & - & + & + & 0 & + & + & + \\ + & + & - & - & - & + & + & - & - & + & + & 0 & + & + & + \end{array}$$

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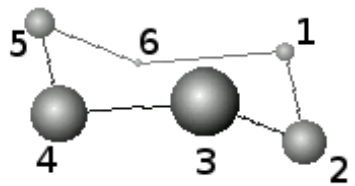

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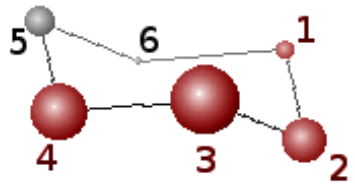
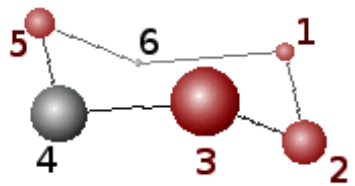


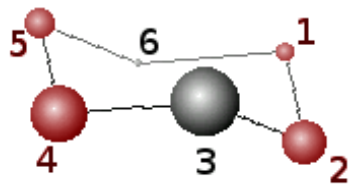
$$\begin{array}{rl} & \begin{array}{cccccccccccccccccccc} 1234 & & & & & 1235 & & & & & 1245 & & & & & 1345 & & & & \end{array} \\ \chi = & + + 0 \; - - + + 0 \; - + + 0 \; + + + \\ \chi = & + + + - - + + + - + + 0 \; + + + \\ \chi = & + + - - - + + - - + + 0 \; + + + \end{array}$$

Partially defined chirotopes



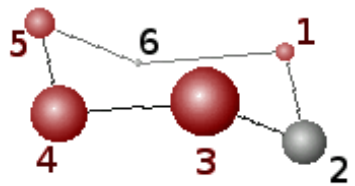
$$\begin{array}{rl} & \begin{array}{cccccccccccccccccccc} 1234 & 1235 & 1245 & 1345 & 2345 & 1236 & 1246 & 1346 & 2346 & 1256 & 1356 & 2356 & 1456 & 2456 & 3456 \end{array} \\ \chi = & + \; + \; 0 \; - \; - \; + \; + \; 0 \; - \; + \; + \; 0 \; + \; + \; + \\ \chi = & + \; + \; + \; - \; - \; + \; + \; + \; - \; + \; + \; 0 \; + \; + \; + \\ \chi = & + \; + \; - \; - \; - \; + \; + \; - \; - \; + \; + \; 0 \; + \; + \; + \end{array}$$

Partially defined chirotopes



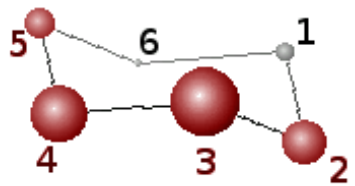
$$\begin{array}{rl} & 1234\ 1235\ 1245\ 1345\ 2345\ 1236\ 1246\ 1346\ 2346\ 1256\ 1356\ 2356\ 1456\ 2456\ 3456 \\ \chi = & +\ +\ 0\ -\ -\ +\ +\ 0\ -\ +\ +\ 0\ +\ +\ + \\ \chi = & +\ +\ +\ -\ -\ +\ +\ +\ -\ +\ +\ 0\ +\ +\ + \\ \chi = & +\ +\ -\ -\ -\ +\ +\ -\ -\ +\ +\ 0\ +\ +\ + \end{array}$$

Partially defined chirotopes



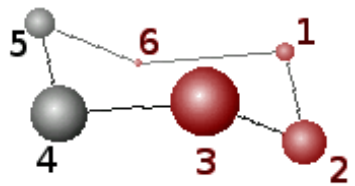
	1234	1235	1245	1345	2345	1236	1246	1346	2346	1256	1356	2356	1456	2456	3456
$\chi =$	+	+	0	−	−	+	+	0	−	+	+	0	+	+	+
$\chi =$	+	+	+	−	−	+	+	+	−	+	+	0	+	+	+
$\chi =$	+	+	−	−	−	+	+	−	−	+	+	0	+	+	+

Partially defined chirotopes



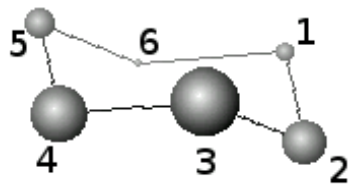
	1234	1235	1245	1345	2345	1236	1246	1346	2346	1256	1356	2356	1456	2456	3456
$\chi =$	+	+	0	−	−	+	+	0	−	+	+	0	+	+	+
$\chi =$	+	+	+	−	−	+	+	+	−	+	+	0	+	+	+
$\chi =$	+	+	−	−	−	+	+	−	−	+	+	0	+	+	+

Partially defined chirotopes



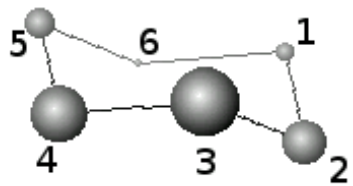
	1234	1235	1245	1345	2345	1236	1246	1346	2346	1256	1356	2356	1456	2456	3456
$\chi =$	+	+	0	−	−	+	+	0	−	+	+	0	+	+	+
$\chi =$	+	+	+	−	−	+	+	+	−	+	+	0	+	+	+
$\chi =$	+	+	−	−	−	+	+	−	−	+	+	0	+	+	+

Partially defined chirotopes



	1234	1235	1245	1345	2345	1236	1246	1346	2346	1256	1356	2356	1456	2456	3456
$\chi =$	+	+	0	−	−	+	+	0	−	+	+	0	+	+	+
$\chi =$	+	+	+	−	−	+	+	+	−	+	+	0	+	+	+
$\chi =$	+	+	−	−	−	+	+	−	−	+	+	0	+	+	+

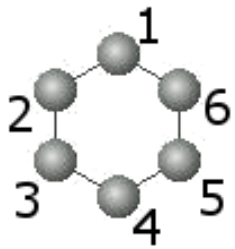
Partially defined chirotopes



	1234	1235	1245	1345	2345	1236	1246	1346	2346	1256	1356	2356	1456	2456	3456
$\chi =$	+	+	0	−	−	+	+	0	−	+	+	0	+	+	+
$\chi =$	+	+	+	−	−	+	+	+	−	+	+	0	+	+	+
$\chi =$	+	+	−	−	−	+	+	−	−	+	+	0	+	+	+

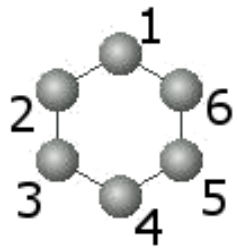
- Partially defined chirotopes give the possibility to classify the conformations in a graduated application-specific manner.

Conformer generation: The example cyclohexane



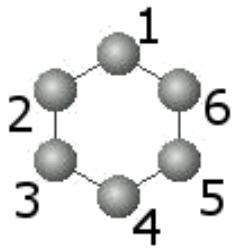
Conformer generation: The example cyclohexane

- The molecular graph has 12 automorphisms.



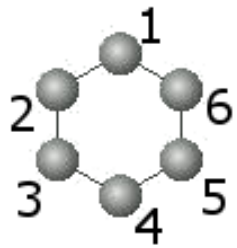
Conformer generation: The example cyclohexane

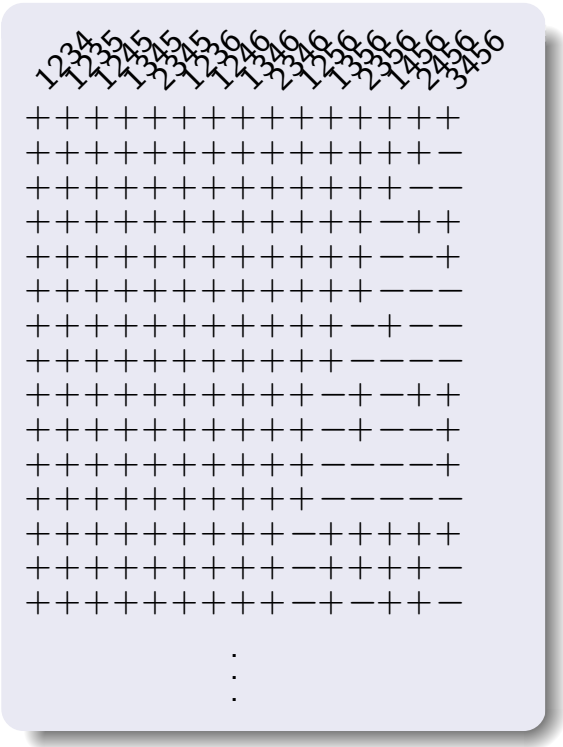
- The molecular graph has 12 automorphisms.
- We assume, that no 4 atoms are in a plane.



Conformer generation: The example cyclohexane

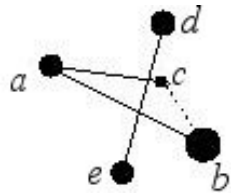
- The molecular graph has 12 automorphisms.
- We assume, that no 4 atoms are in a plane.
- We get 386 chirotopes.

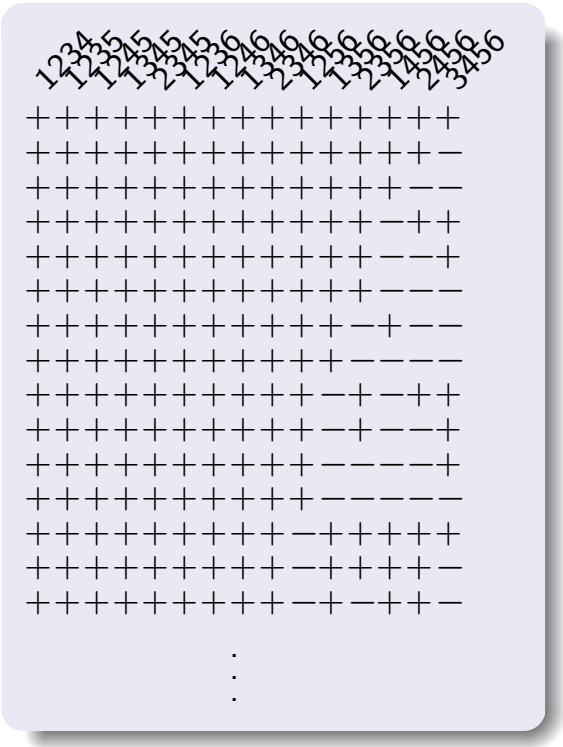




Conformer generation: The example cyclohexane

- The molecular graph has 12 automorphisms.
- We assume, that no 4 atoms are in a plane.
- We get 386 chirotopes.
- Excluding unfeasable radon partitions: 162





Conformer generation: The example cyclohexane

- The molecular graph has 12 automorphisms.
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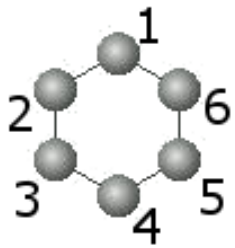
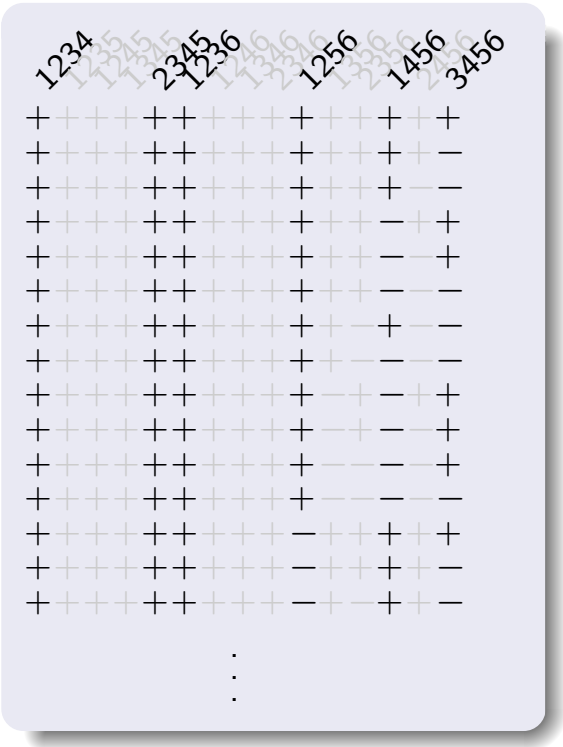
- Restricting to quadrupels corresponding to a gauche/anti-situation:





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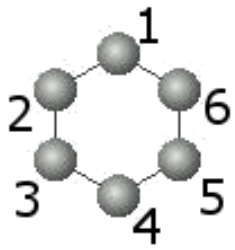

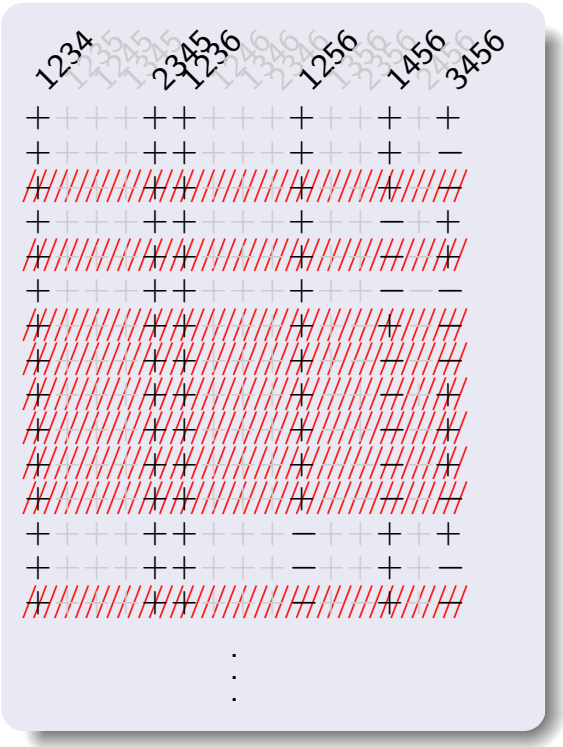

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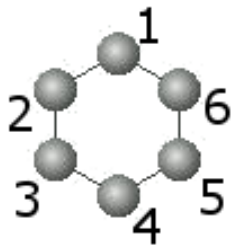

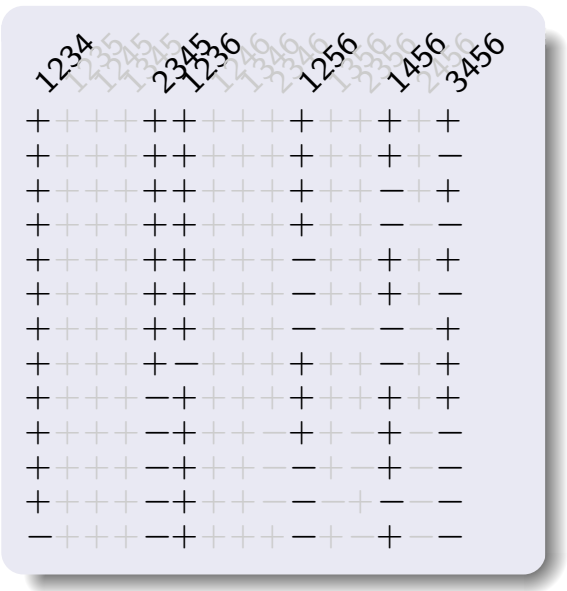

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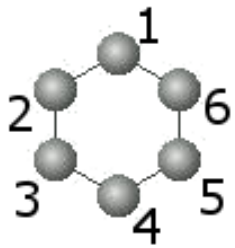

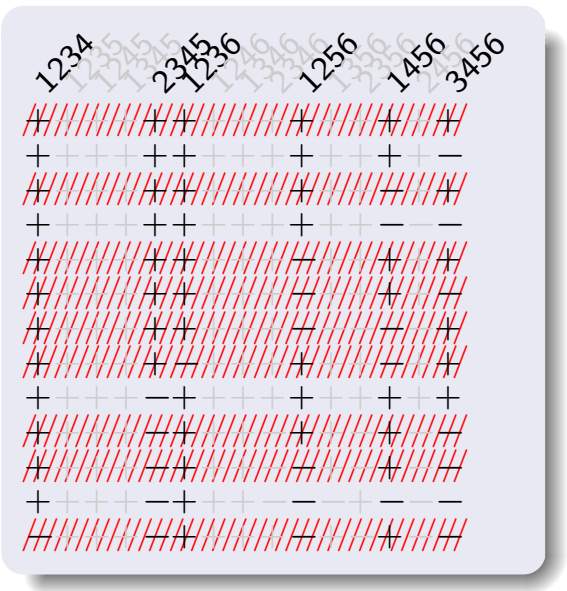

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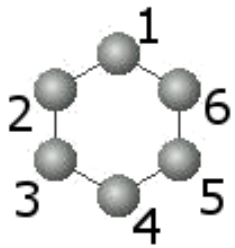

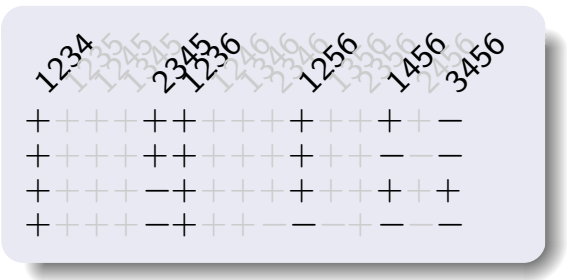

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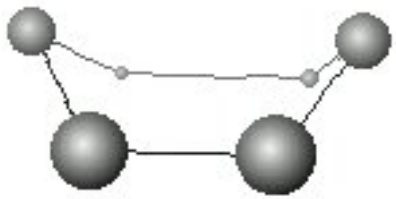
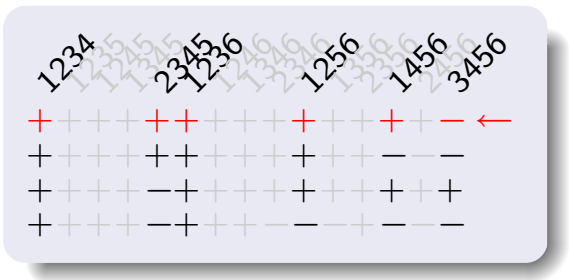
  - boat form (a “sattle point”)





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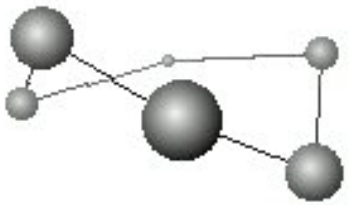

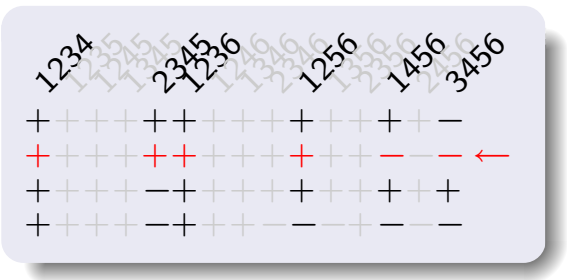

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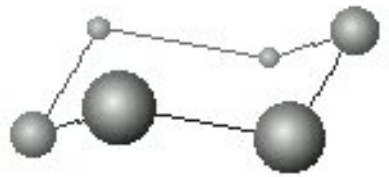
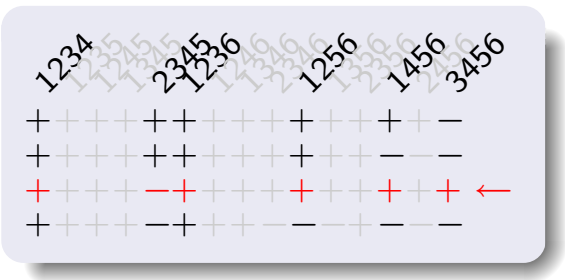
- Restricting to quadrupels corresponding to a gauche/anti-situation: 13
- Conformation as local minima of an energy function were found for: 4
  - boat form (a “sattle point”)
  - twist form
  - chair form





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- Restricting to quadrupels corresponding to a gauche/anti-situation: 13
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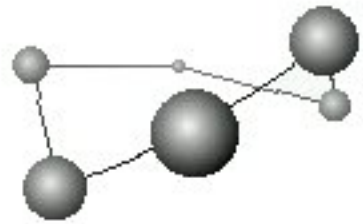
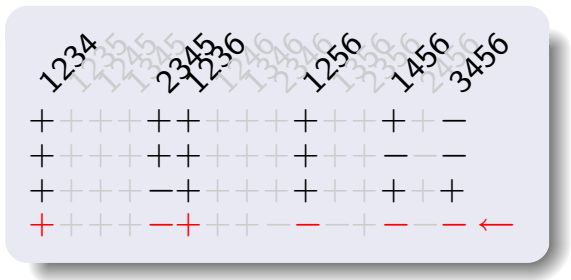
  - twist form
  - chair form
  - twist form (enantiomere)





Thanks

Thank You!